



Direct 3D Phase-Retrieval and Tomographic Reconstruction of Coherent Diffraction Patterns

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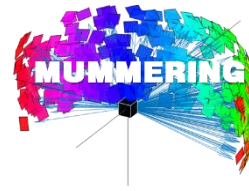
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- **X-ray phase contrast nano-tomography of 3rd generation solar cells**
- **Resonant X-ray Ptychographic Tomography of CZTS Solar Cells**
- **Nano-scale 3D reconstruction of phase contrast X-ray projections**
- **High Resolution X-ray Diffraction Contrast Tomography**
- **In situ structural characterization of multilayer formation during large-scale processing of 3rd generation solar cells**
- **Roll-to-roll (R2R) coating of 3rd generation solar cells with optimal nanostructure**
- **Photovoltaic CZTS absorber layer research**
- **Modelling of ultrafast scattering experiments probing electronic dynamics in solar cells**
- **Mesoscale modelling of morphologies, charge carrier generation, and charge transport in 3rd generation solar cells**

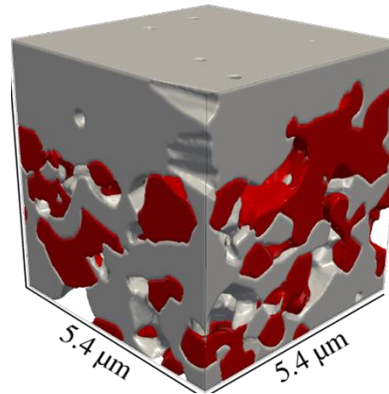
Energy Research at DTU and the need for high-resolution microscopy

Batteries



DTU Inside

Fuel Cells



Courtesy of Salvatore De Angelis

Solar Cells

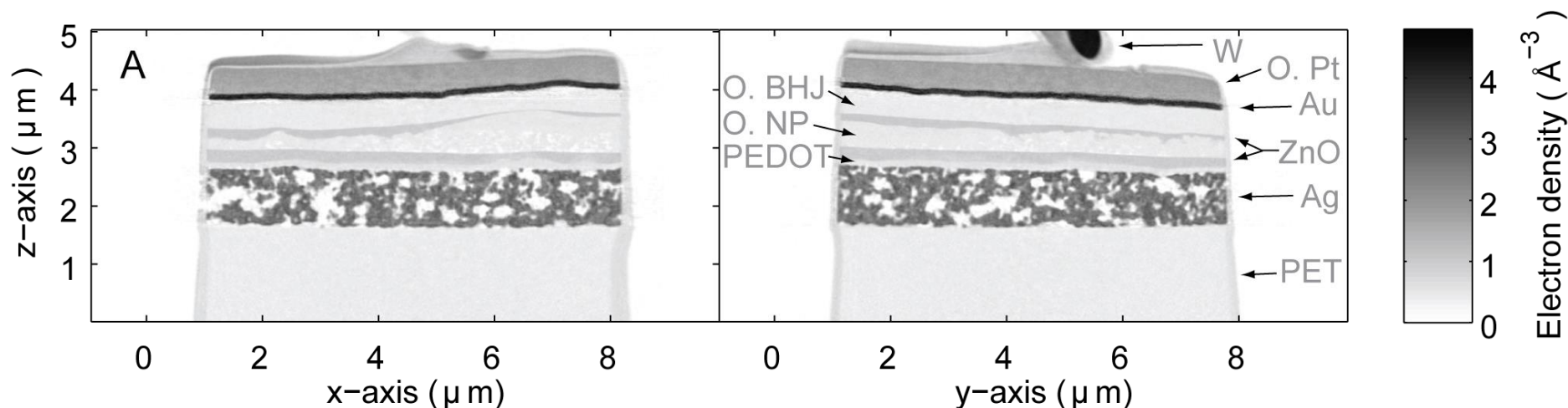
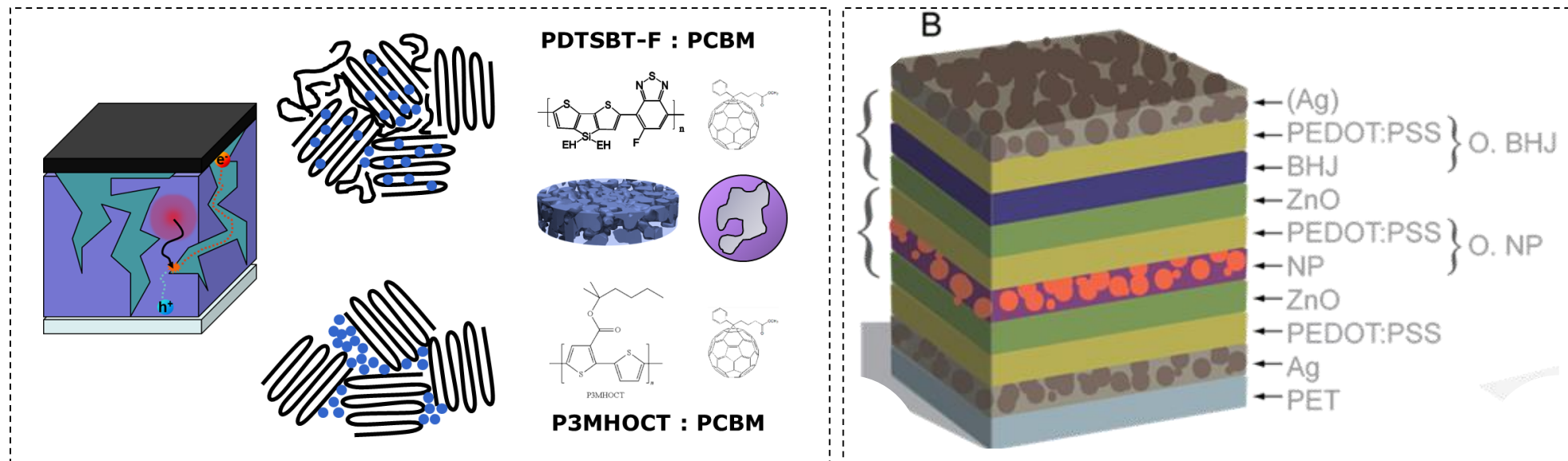


DTU Inside

The performance, efficiency, stability and lifetime of numerous engineering materials and biological systems are largely defined by their internal structure down to the **micro- and nanoscale**.

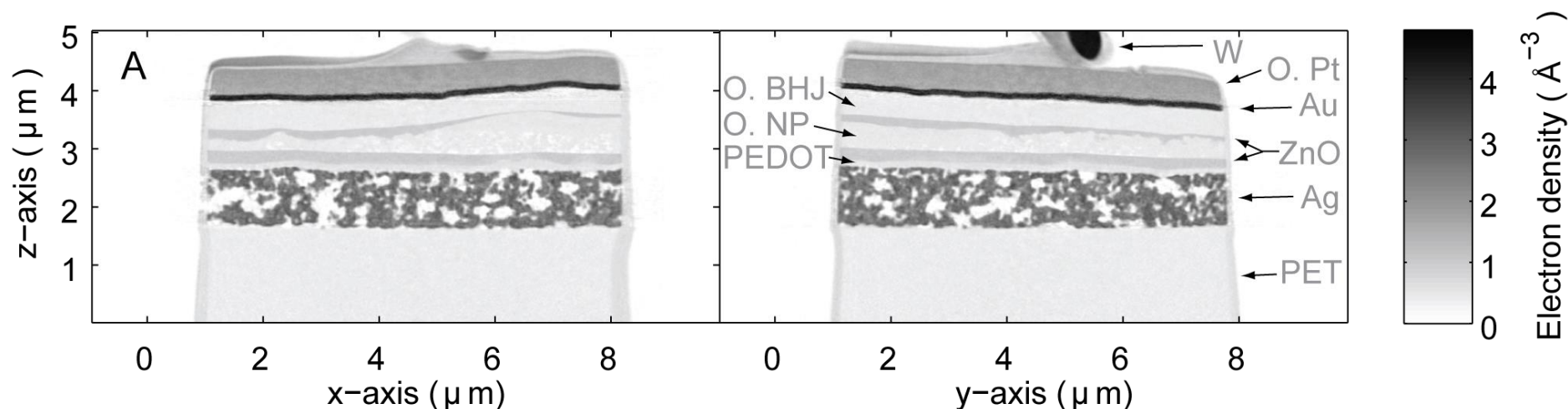
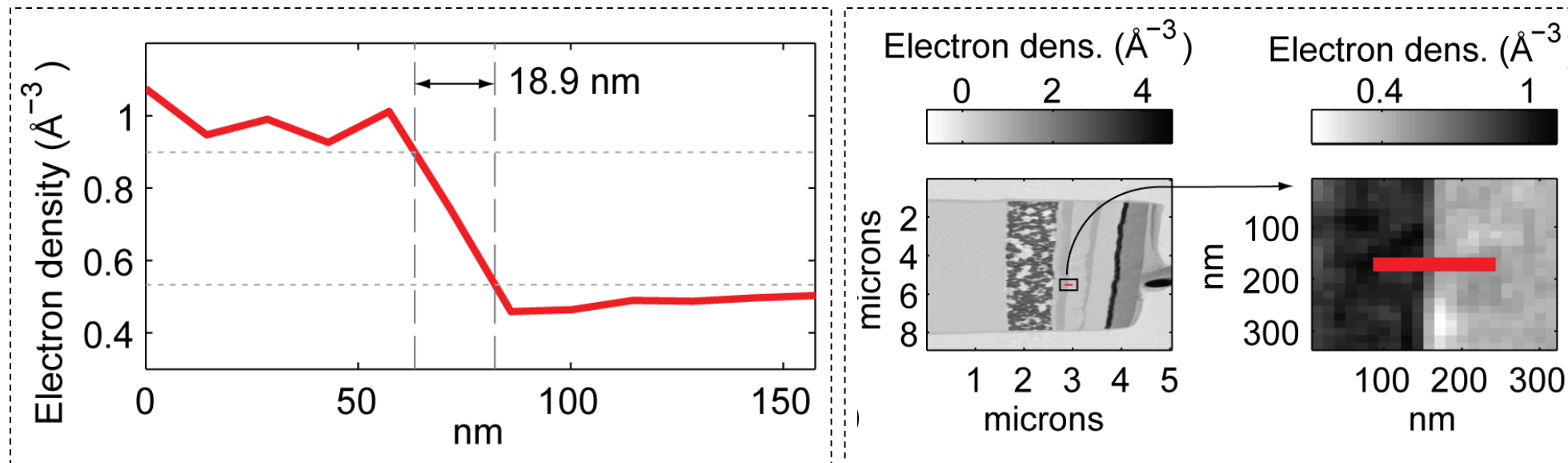
Energy Research at DTU

and the need for high-resolution microscopy



Energy Research at DTU

and the need for high-resolution microscopy

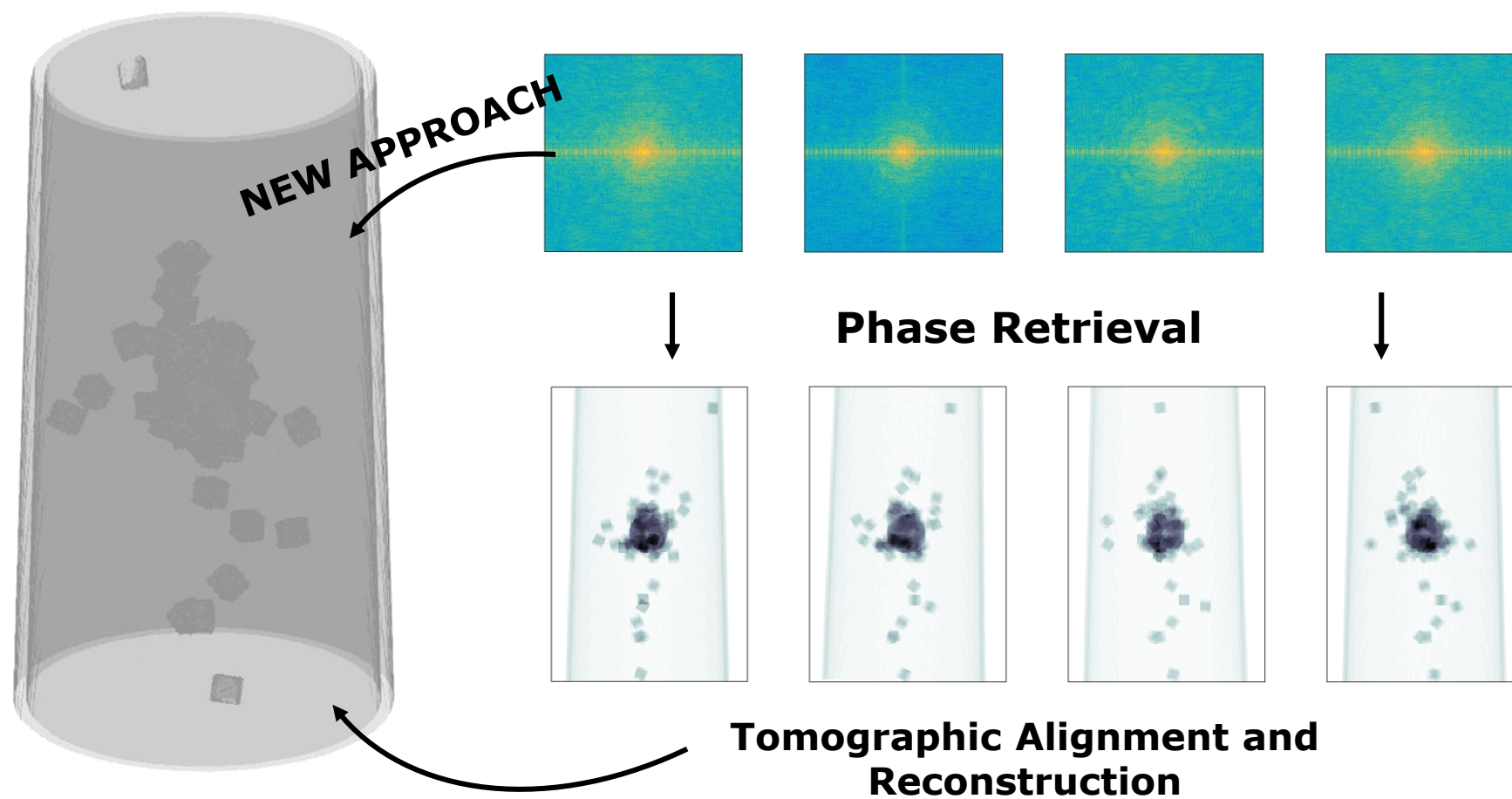


Direct 3D Phase-Retrieval and Tomographic Reconstruction of Coherent Diffraction Patterns

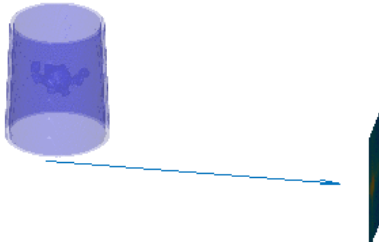
Tiago João Cunha Ramos

Jens Wenzel Andreasen

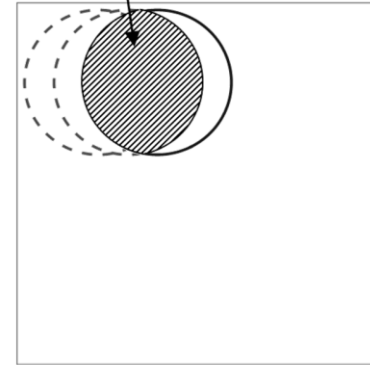
Azat M. Slyamov



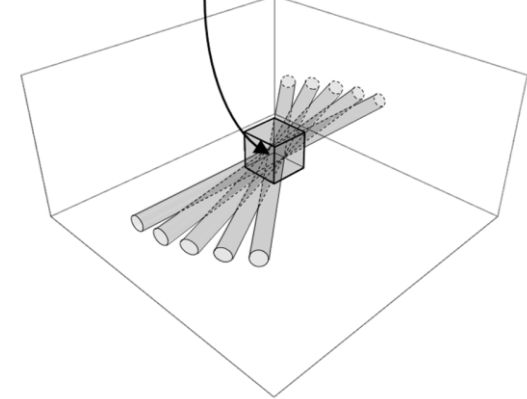
2D vs 3D



Probe overlap in 2D Ptychography



Probe overlap in 3D Ptychography

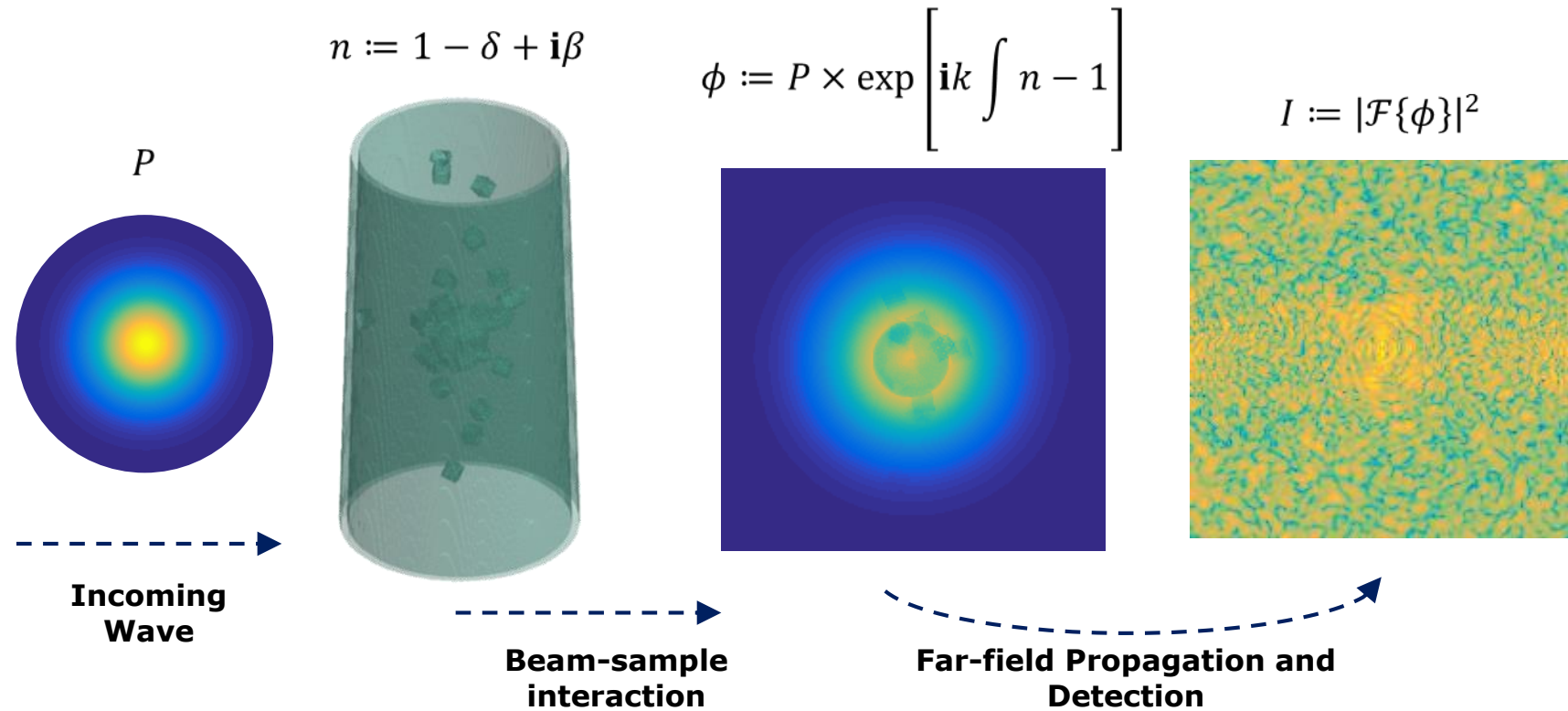


Advantages:

- Relaxed overlapping conditions.
- Reduction in acquired data.
- Faster experiments.
- Less radiation damage.

Gürsoy, Doğa. "Direct coupling of tomography and ptychography." *Optics letters* 42.16 (2017): 3169-3172.

Forward Model



$$I := \left| \mathcal{F} \left\{ P \times \exp \left[\mathbf{i}k \int n - 1 \right] \right\} \right|^2$$

- **Non-linear**
- **Ill-posed**
- **Non-differentiable**
- **Complex arguments**

Ramos, Tiago, et al. "Direct three-dimensional tomographic reconstruction and phase retrieval of far-field coherent diffraction patterns." *Physical Review A* 99.2 (2019): 023801.

Forward Model: $n \rightarrow I$

$$n' = n - 1 = -\delta + i\beta$$

Attenuation and Phase-shift:

$$p^{out} = p^{in} \cdot \exp[ik\mathcal{R}_{\Theta}(n')]$$

Free-space far-field propagation

$$p^{out,propagated} = \mathcal{F}\{P \cdot \exp[ik\mathcal{R}_{\Theta}(n')]\}$$

Intensity Detection

$$I_{\Theta}^f = F(n') = |\mathcal{F}\{P \cdot \exp[ik\mathcal{R}_{\Theta}(n')]\}|^2$$

n – Complex refractive index
 δ – Refractive part of refractive index
 β – Absorptive part of refractive index
 i – Imaginary unit
 P – Probe function

Quadratic Approximation log-likelihood function:

$$l(\mu_N, \sigma_N^2, x) = -\frac{1}{2\sigma_N^2} \sum_i (x_i - \mu_N)^2$$

Maximizing log-likelihood = Minimizing negative log-likelihood

$$\min_{n'} f(n') = \frac{1}{2} \sum_i \left(\frac{I_{\Theta_i}^f(n') - I_{\Theta_i}^m}{\sigma_i} \right)^2 \quad \sigma \approx \sqrt{I_{\Theta}^m + \epsilon}$$

Linearize Cost-function:

$$f(n' + \Delta n') \approx f(n') + \nabla f(n') \Delta n' + \frac{1}{2} \Delta n'^* \nabla^2 f(n') \Delta n'$$

$$\nabla f(n') = J(n')^* r(n'), \quad \nabla^2 f(n') \approx J(n')^* J(n')$$

Compute reconstruction update: $h_{n'}$

$$(J^{*[l]} J^{[l]} + \lambda_{lm} \mathbf{I}) h_{n'}^{[l]} = -J^{*[l]} r^{[l]}$$

Update Solution:

$$n'^{[l+1]} = n'^{[l]} + h_{n'}^{[l]}$$

Enforce known Constraints

$$n'^{[l]} = -\delta^{[l]} + i\beta^{[l]} = \min(-\delta^{[l]}, 0) + i \max(\beta^{[l]}, 0).$$

Jacobian and its adjoint for tomographic reconstruction

$$\begin{aligned}
 J\left(n'^{[l]}\right) h_{n'}^{[l]} &= \frac{1}{\sqrt{I_{\Theta}^m} + \epsilon} 2\Re \left[\overline{\left(\mathcal{F} \{ P \cdot \exp[\mathbf{i}k\mathcal{R}_{\Theta}(n'^{[l]})] \} \right)} \mathcal{F} \left\{ \mathbf{i}Pk \cdot \exp[\mathbf{i}k\mathcal{R}_{\Theta}(n'^{[l]})] \mathcal{R}_{\Theta}(h_{n'}^{[l]}) \right\} \right] \\
 &= \frac{1}{\sqrt{I_{\Theta}^m} + \epsilon} 2\Re \left[\overline{(\Psi_{\Theta}^{[l]})} \mathcal{F} \left\{ (\mathbf{i}k\psi_{\Theta}^{[l]}) \mathcal{R}_{\Theta}(h_{n'}^{[l]}) \right\} \right] \\
 J\left(n'^{[l]}\right)^* h_g^{[l]} &= 2\mathcal{R}_{\Theta}^* \left[\overline{\mathbf{i}Pk \cdot \exp[\mathbf{i}k\mathcal{R}_{\Theta}(n'^{[l]})]} \mathcal{F}^{-1} \left\{ \frac{1}{\sqrt{I_{\Theta}^m} + \epsilon} \left(\mathcal{F} \{ P \cdot \exp[\mathbf{i}k\mathcal{R}_{\Theta}(n'^{[l]})] \} \right) \Re[h_g^{[l]}] \right\} \right] \\
 &= 2\mathcal{R}_{\Theta}^* \left[\overline{(\mathbf{i}k\psi_{\Theta}^{[l]})} \mathcal{F}^{-1} \left\{ \frac{\Psi_{\Theta}^{[l]} h_g^{[l]}}{\sqrt{I_{\Theta}^m} + \epsilon} \right\} \right]
 \end{aligned}$$

Jacobian and its adjoint for Probe function reconstruction

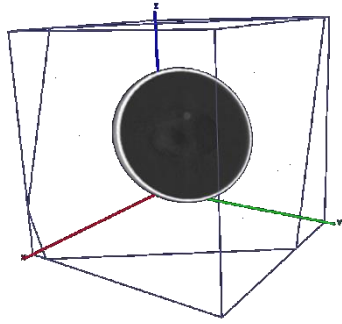
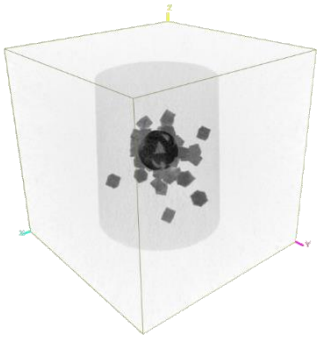
$$\begin{aligned}
 J(P^{[l]}) h_P^{[l]} &= \frac{1}{\sqrt{I_{\Theta}^m} + \epsilon} 2\Re \left[\overline{(\Psi_{\Theta}^{[l]})} \mathcal{F} \{ O_{\Theta}^{[l]} h_P \} \right] \\
 J(P^{[l]})^* h_g^{[l]} &= 2\overline{O_{\Theta}^{[l]}} \mathcal{F}^{-1} \left\{ \frac{\Psi_{\Theta}^{[l]} h_g^{[l]}}{\sqrt{I_{\Theta}^m} + \epsilon} \right\}
 \end{aligned}$$

n – Complex refractive index
 δ – Refractive part of refractive index
 β – Absorptive part of refractive index
 i – imaginary unit
 P – Probe function

\mathcal{F}_2 – 2D Fourier Transform
 \mathcal{F}_2^* – 2D Inverse Fourier Transform
 $F(N)$ – Forward Model Operator
 $F'[N]$ – Fréchet derivative
 $F'[N]^*$ – Adjoint of Fréchet derivative

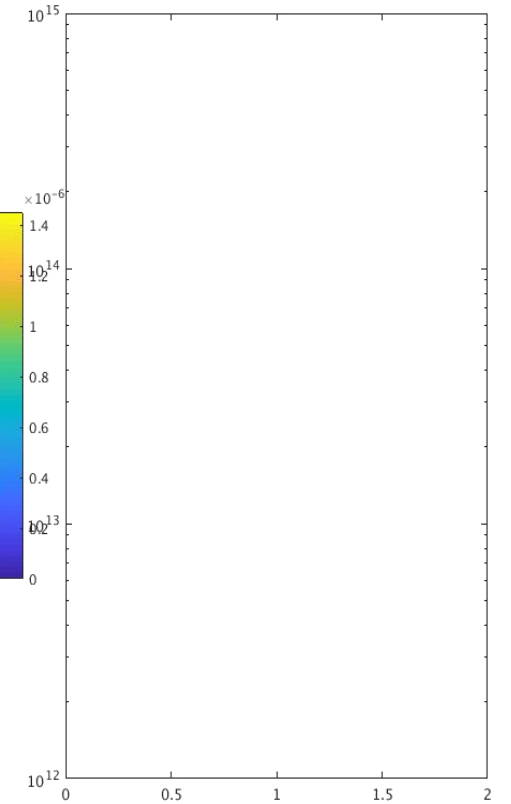
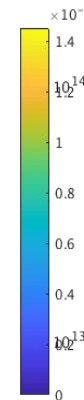
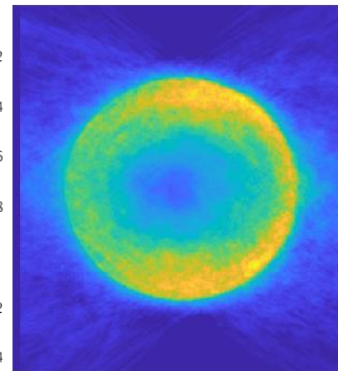
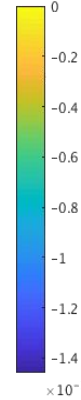
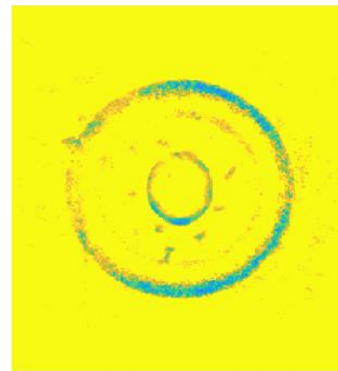
\Re – Real part (element-wise operator)
 \mathcal{R} – Radon transform
 \mathcal{R}^* – Back projection
 h_N – Increment on N
 g – Increment on *diffraction patterns*

Tomographic slice on reconstructed refractive indexes (simulation)

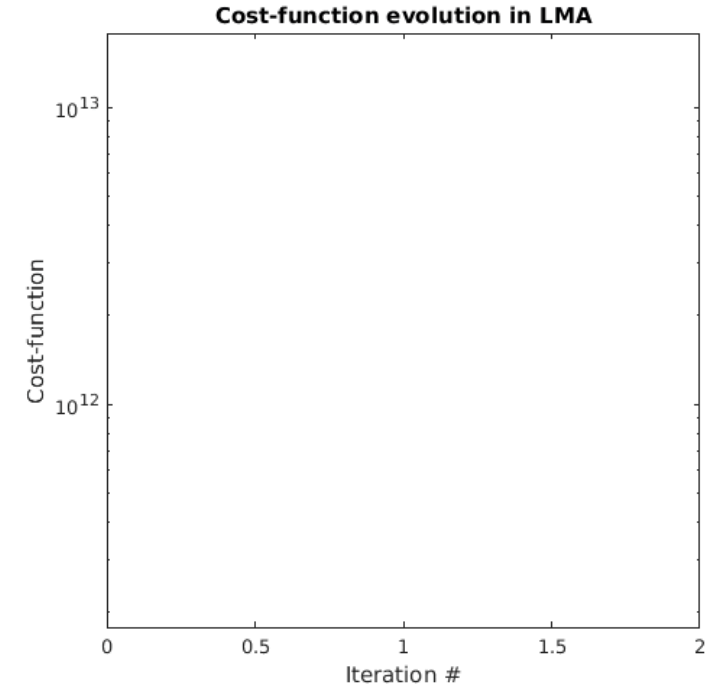
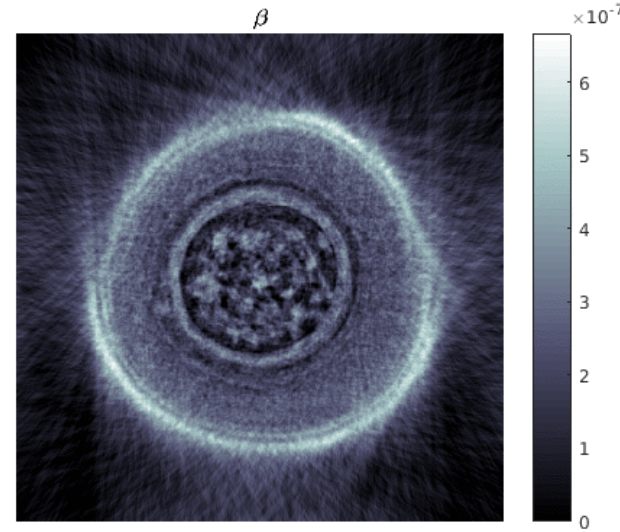
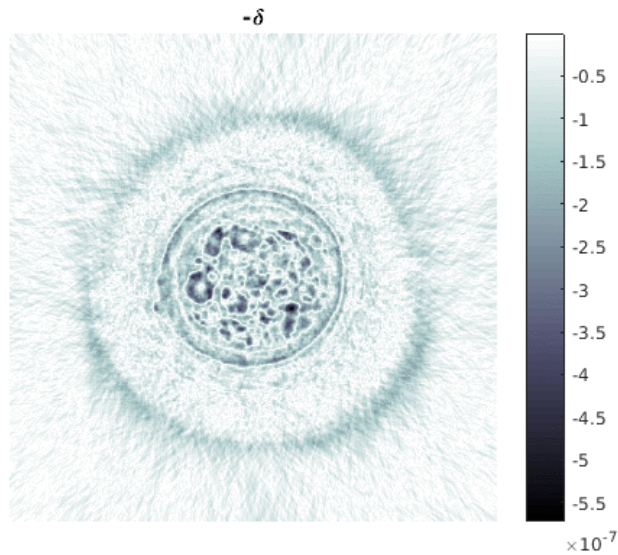


Simulation results:

- 300^3 voxels volume
- Detector 100^2 Pixels
- 3200 Diffraction Patterns
 - 200 Angles
 - 16 Expos. per angle



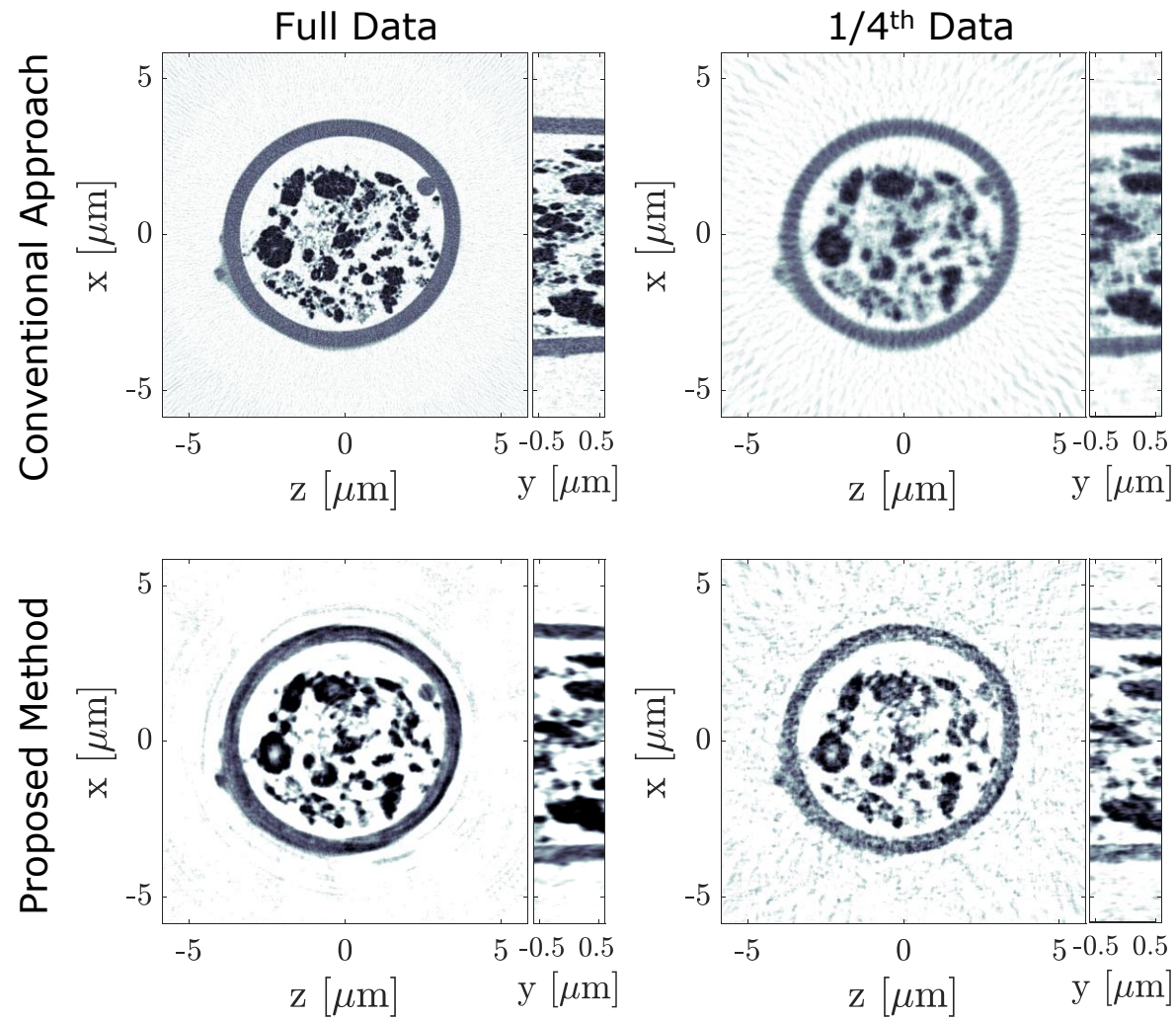
Tomographic slice on reconstructed refractive indexes (experimental data)



Results on real-data reconstruction

- 200 Projection angles
- 176 scanning points/projection
- Effective detector size – 600x600 Pixels
- Pixel size -14.3 nm
- Volume $1000^3 \sim 16$ GB (double precision)
- >35000 diffraction patterns ~ 100 GB (double precision)

Real data reconstruction



Reconstruction:

- Only 20 iterations LMA
- Non-negativity constraint
- Diffraction patterns *cropped* to half size

Challenges

- High sensitivity to initial guess of the probe
- No real-space alignment
- High computational costs and memory requirements

Possible solutions

- Initial reconstruction of the probe at a given angle
- Hardware solution for high precision alignment
- Multiple GPUs system

Thank you for your attention!